Basic Energy Sciences Update

Basic Energy Sciences Advisory Committee Meeting September 24, 2024

> Andy Schwartz and Gail McLean Office of Basic Energy Sciences



https://science.osti.gov/



New Quantum Information Sciences Program Manager Chemical Sciences, Geosciences and Biosciences Division



Dr. Marat Valiev

Expertise

- Development and application of high-performance molecular simulation methods to describe chemical transformations in chemical & biological systems
- Advancing new interdisciplinary approaches for understanding how atomic-level quantum information translates to the macroscopic scale using concepts from quantum field theory, statistical mechanics, and quantum chemistry

- Joined BES in April 2024 as the program manager for CSGB Quantum Information Sciences
- Computational Scientist at the Pacific Northwest National Laboratory (PNNL) where he was a Team Lead for Systems Modeling and Computational Sciences and later for Basic and Applied Molecular Foundations
- Detailee with the Condensed Phase and Interfacial Molecular Science (CPIMS) Program in CSGB
- Ph.D. in Condensed Matter Physics and M.S. in Physics from the University of Connecticut

New Cross-Office of Science (SC) Coordination Program Manager Collaborative Research Division (EPSCoR, RENEW, FAIR)



Dr. Tim Kidd

Expertise

- Experimental condensed matter and materials physics
- Nanocellulose and 2D metallic interfaces, electronic properties of layered materials
- Undergraduate education

- Joined BES in June 2024 as the program manager for Cross-Office of Science (SC) Coordination which includes management of the RENEW, FAIR, and EPSCoR programs
- Professor of physics at the University of Northern Iowa where he worked extensively with undergraduate students in his research program that spanned areas of experimental condensed matter and materials physics
 - Developed a suite of new courses to support education in the fields of robotics and nanoscience
 - Elected leadership: chair of the faculty, faculty senate, and regional zone councilor for Society of Physics Students
- Ph. D. in Physics and B.S. in Engineering Physics from the University of Illinois at Urbana-Champaign

New QIS/AMOS Program Manager & Quantum Liaison for the National Quantum Coordination Office Chemical Sciences, Geosciences and Biosciences Division



Dr. Hilary Hurst

Expertise

- Theoretical condensed matter and AMO physics
- Many-body atomic physics and quantum information science
- Quantum control for open systems

- Joined BES in August 2024 on temporary assignment through the Intergovernmental Personnel Act as a program manager for Quantum Information Sciences as well as for Atomic, Molecular and Optical Sciences
- Also serves as the Quantum Liaison for the National Quantum Coordination Office, White House Office of Science and Technology Policy (OSTP), where she coordinates workforce development and outreach efforts in support of the National Quantum Initiative
- Assistant Professor in the Physics & Astronomy Department of San Jose State University
- Ph.D. in Physics, Univ of Maryland; M.S. in Theoretical Physics & Applied Mathematics, Univ of Cambridge

New AAAS Science & Technology Policy Fellow Basic Energy Sciences



Dr. Aaron Stone

Expertise

- Experimental inorganic chemistry; nanomaterials; photocatalysis
- Metal-organic frameworks and quantum dot synthesis and application
- Research collaboration; science communication
- International energy issues

- ORISE Fellow in DOE's Office of International Affairs (2023-2024)
- Ph.D. in Chemistry from Northwestern University (Hupp and Weiss Groups; 2023)
- Thrust Coordinator, Center for Light Energy Activated Redox Processes (2019-2020)
- B.A. in Chemistry from Wesleyan University (2018)

BES is Hiring! Positions currently open:

Geosciences Program Manager in the CSGB Division

- https://www.usajobs.gov/job/783518800; Open until September 30
- Open to the public (U.S. citizens, nationals)
- The Program Manager will determine scientific focus and direction of a broad portfolio of fundamental geochemistry and geophysics research, prepare calls for proposals, organize independent peer reviews, recommend funding allocations, organize Principal Investigator meetings, serve as a liaison on committees, and assess scientific progress of the research portfolio.

Project Program Manager in the SUF Division

- https://www.usajobs.gov/job/783518800; Open until September 30
- Open to the public (U.S. citizens, nationals)
- The Project Program Manager will help manage the Division's portfolio of scientific user facility construction and upgrade projects, act as a recognized technical authority and expert in the development and management of the construction project portfolio, and serve as a subject matter expert for all aspects of project management, particularly for user facility upgrade/construction projects, following relevant DOE policies, procedures, and Orders.

Nominations Requested: Collaborative Research Division Director

- BES is requesting help in identifying candidates for the Collaborative Research Division Director, which is a Career position in the Senior Executive Service.
- The Collaborative Research Division supports:
 - Multidisciplinary, multi-institution team research such as Energy Frontier Research Centers (EFRCs), Energy Innovation Hub programs, and Energy Earthshot Research Centers
 - Cross-SC diversity and technology coordination activities such as DOE EPSCOR, RENEW and FAIR
- The Collaborative Research Division Director will be responsible for overall division management, including strategic planning; budget formulation and execution; program integration with SC activities and other DOE offices; interagency and international liaison; and management of the Division staff
- Please send nominations to both Andy Schwartz (<u>Andrew.Schwartz@science.doe.gov</u>) and Mariam Elsayed (<u>Mariam.Elsayed@science.doe.gov</u>) with the individual's name, position, organization information, and email address by **October 4, 2024.**
 - Each nominated individual will be sent a letter providing information on the position and how to apply and will be encouraged to submit an application.



Call for Nominations: Collaborative Research Division Director, Office of Basic Energy Sciences

FY 2024 BES Funding Opportunities

- Annual Open Solicitation: Supports grants for research in the topical areas supported by the Office of Science. Accepts applications continuously.
- EPSCoR-State/National Laboratory Partnerships. Supports collaborations between EPSCoR-eligible institutions and DOE national laboratories on fundamental, early-stage energy science research.
 Awards announced Aug. 22, 2024 \$36M for 39 awards in 19 states
- Computational Materials Sciences Exploratory Research at the Exascale: Computational codes and associated databases for materials design with advanced functionalities. Awards announced August 28, 2024 - \$14M for 4 DOE lab awards.
- Energy Frontier Research Centers: Supports multi-disciplinary, multi-institutional centers to enable transformative advances in energy-relevant basic science, emphasizing QIS, microelectronics, transformative manufacturing, and environmental management. Awards announced Sept. 4, 2024 - \$118M for 10 new and renewing Centers led by 6 universities and 4 DOE Laboratories with 65 additional partner institutions.
- Annual Early Career FOA: Supports outstanding scientists early in their careers in research areas supported by the Office of Science; all BES core research areas and facilities capabilities research.
 Awards announced Sept. 10, 2024 - \$58M for 46 BES awards at 32 unique universities and 8 unique DOE Lab.
 - RENEW, FAIR: Supports efforts to broaden participation within the SC research community through training opportunities leveraging the DOE complex and direct research support at non-R1 MSIs and ERIs (incl. DOE lab and R1 MSI partners).
 Proposals under review. Announcements anticipated early FY 2025.



★ Details on subsequent slides

Computational Materials Science – Exploratory Research at the Exascale

- Scope: Produce widely applicable, validated public-access community codes and associated databases for functional materials that leverage the exascale software stack and ECP work.
- Requirements: Fully integrated, multi-investigator teams led by DOE labs and exascale-ready software
- Topics: (1) Computational discovery and design of functional materials with unique physical properties; (2) computational modeling of emergent and ordered magnetic, superconducting, and/or ferroelectric phases, including their dynamics.
- <u>Awards</u> \$14M for 4 new and renewal awards led by 4 DOE labs with 12 partner institutions
 - Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM) | Lead: Steven Louie
 – Lawrence Berkeley National Laboratory (Renewal)
 - Center for Predictive Simulation of Functional Materials (CPSFM) | Lead: Paul Kent Oak Ridge National Laboratory (Renewal)
 - Accelerating the discovery and design of advanced functional materials using AI/ML and exascale computing | Lead: Cai-Zhuang Wang – Ames National Laboratory (New)
 - Navigating the Design Space of Heterostructures: Advancing Functionality of Modeling for 2D Materials and Transition Metal Oxides | Lead: Eric Bylaska - Pacific Northwest National Laboratory (New)

Energy Frontier Research Centers

- Topics:
 - Renewals: (1) Transformative manufacturing; (2) Quantum information science; (3) Environmental management
 - New: (1) Co-design of materials and processes to revolutionize microelectronics and/or QIS fabrication;
 (2) Environmental management
- Awards: 10 new and renewal awards led by 6 universities and 4 DOE Labs (75 partner institutions)
 - A Center for Power Electronics Materials and Manufacturing Exploration (APEX) | Lead: Nancy Haegel NREL (new)
 - Quantum Photonic Integrated Design Center (QuPIDC) | Lead: Libai Huang Purdue University (new)
 - Center for Plastics Innovation (CPI) | Lead: LaShanda Korley University of Delaware (renewal)
 - Ion Dynamics in Radioactive Environments and Materials (IDREAM) | Lead: Carolyn Pearce PNNL (renewal)
 - Institute for Cooperative Upcycling of Plastics (iCOUP) | Lead: Aaron Sadow Ames National Laboratory (renewal)
 - Center for Energy Efficient Magnonics (CEEMag) | Lead: Yuri Suzuki SLAC (new)
 - Center for 3D Ferroelectric Microelectronics Manufacturing (3DFEM2) | Lead: Susan Trolier-Mckinstry Pennsylvania State University (renewal)
 - Center for Molecular Quantum Transduction (CMQT) | Lead: Michael Wasielewski Northwestern University (renewal)
 - EFRC for Quantum Sensing and Quantum Materials (QSQM) | Lead: Peter Abbamonte University of Illinois Urbana Champaign (renewal*)
 - Ultra Materials for Resilient, Smart Electricity Grid (ULTRA) | Lead: Arizona State University (renewal*)

* Two-year transition

Early Career Research Program (ECRP)

Location of all 466 BES ECRP Awards from 2010 - 2024





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Location of 46 BES ECRP Awards in 2024

BES ECRP Awards in 2024

- 22 states and 40 unique institutions
- 5 new institutions (since program inception)
- 4 awards to EPSCoR institutions
- 8 HSI awards

Batteries and Energy Storage Hub Awards (Announced September 2024)

Energy Storage Research Alliance (ESRA)

Scope: Establish science foundation to achieve unprecedented molecular level control of reactivity, ion selectivity, and directional transport for long-duration grid storage and heavy-duty transportation

Lead Institution: Argonne National Lab (14 national lab and university partner institutions) Budget: up to \$62.5M over 5 years

Aqueous Battery Consortium (ABC)

Scope: Establish the scientific foundation for large-scale deployment of aqueous earth-abundant (Zn, Fe, Mn) batteries for long-duration energy storage for the grid

Lead Institution: Stanford University (13 national lab and university partner institutions) Budget: up to \$62.5M over 5 years



Advanced Microelectronics Lab Call

- Microelectronics Science Research Centers will comprise a network of multiple multidisciplinary team awards
 - Perform mission-driven research to address foundational challenges in the design, development, characterization, prototyping, demonstration, and fabrication of microelectronics
 - Each Center will be made up of individual team awards that focus on research required for a common Center goal
 - Teams will include researchers from universities, national laboratories, and industry
 - Lab Call released May 8, 2024; awards to be announced early FY 2025.
- Continued coordinated SC support for multi-disciplinary research to accelerate the innovation and advancement of microelectronic technologies in a co-design ecosystem
 - Includes fundamental research on materials, chemistries, processing, isotopes, devices, systems, architectures, algorithms, and software
 - Builds on capabilities at SC user facilities for computation, fabrication, and characterization
 - Provides foundational knowledge for development of next-generation technologies in computing, communications, sensing, and power
- Basic research in microelectronics complements later-stage investments being made by other agencies through the CHIPS Act









Microelectronics at the Department of Long Consultance Operation In Princ LUD workshops

Department of Energy Office of Science Fusion Energy Sciences Workshop Plasma Science for Microelectronics Nanofabrication





Energy.gov/science

FY 2025 FOA: EPSCoR Implementation Awards

- Solicitation Scope (<u>DE-FOA-0003444</u> Issued September 12, 2024):
 - Enhance S&T capabilities of designated jurisdictions to conduct nationally competitive research relevant to DOE's science and energy missions; promote geographic and institutional diversity, including training of scientists and engineers in geographically underserved jurisdictions.
- Program Planning/Context:
 - On behalf of DOE, BES publishes the EPSCoR Implementation Award FOA biennially
- Program Coordination:
 - Coordination across DOE, with ~10% matching funds from participating Offices
 - Since FY 2023, EPSCoR funds are distributed among SC Offices: \$25M BES, \$2M in ASCR, BER, FES, HEP & NP (\$35M Total).
- Planned application requirements:
 - Eligible Institutions: Using NSF criteria (<u>https://new.nsf.gov/funding/initiatives/epscor/epscor-criteria-eligibility</u>) colleges/universities in 28 jurisdictions
 - Estimated award size/duration: Up to \$1,500/2,500K per year for new/renewal awards with a duration of two years and up to two 2-year renewal options for new awards.
 - Funding: Up to \$35M in FY 2025 (pending appropriation)
 - Pre-applications will be required. Limitation of 1 pre-application and applications per institution per topical area (by SC program and Technology Offices, with EERE divided into three sectors). 1 application per lead PI.

SC Energy Earthshots Initiative (ASCR, BES, BER)

- Fundamental research to accelerate breakthroughs required to address challenges for the stretch goals of the DOE Energy Earthshots
 - The first six Earthshots are supported with SC awards announced in FY 2023. Two additional Earthshots were announced in FY 2023: Affordable Home Energy and Clean Fuels & Products
- Energy Earthshot Research Centers (EERCs) established in FY 2023

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- Advances foundational knowledge and state-of-the-art capabilities in experimental, theoretical, and computational sciences needed to realize new approaches and solutions.
- Large, multi-investigator, multi-disciplinary national laboratory-led teams.
- Close coordination with the Energy Technology Offices and existing research consortia/demonstration projects to enhance cross-office research cooperation.

• EERCs are complemented by small group awards focused on use-inspired fundamental

research to address knowledge gaps that limit achievement of the Energy Earthshot goals **Hydrogen Shot** Long Duration Storage Shot **Carbon Negative Shot Clean Fuels and Products** ******* CO₂ Reduce storage in 1 decade costs by 90%*... .. in storage systems <100 Dollars 1 Ton 1 Decade 85% Reduction 2035 1 Dollar 1 Kilogram 1 Decade That deliver 10+ hours *from a 2020 Li-Ion baseline of duration .S. DEPARTMENT OF Office of



Affordable Home Energy Shot

Science Summit for Energy Earthshot Innovation

- **Goal:** Opportunity for multi-disciplinary teams funded in ASCR, BES, and BER to collaborate, engage, and discuss foundational research needed to support the DOE Energy Earthshot portfolio
- Held September 4-5th, 2024 in Rockville, MD
- Over 200 attendees

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- Energy Earthshot Research Centers (EERCs)
- Science Foundations for the Energy Earthshots (SFEEs)
- Bioenergy Research Centers (BRCs)
- Energy Frontier Research Centers (EFRCs)
- Mathematical Multifaceted Integrated Capability Centers (MMICCs)
- ASCR Software Stewardship projects
- Fuels from Sunlight Energy Innovation Hubs
- User Facilities and other SC Resources
- S4, SC PMs & upper management, DOE Technology Offices
- Agenda included plenary talks, poster sessions, and discussionbased breakout sessions on DOE Energy Earthshot Research and Cross-cutting Foundational Science topics





)earthshot





Facilities Project Updates and Major Milestones

- Advanced Photon Source Upgrade (ANL): Installation of the multi-bend achromat storage ring completed March 2024, with first light in June 2024 and a return of users in July 2024. Beamline installation and commissioning is ongoing.
- Proton Power Upgrade (ORNL): Operating at 1.7MW, 1.3 GeV since neutron production resumed in July 2024. Project delivered neutrons for the user program in July 2024. Planning underway for the Critical Decision (CD)-4 (Approve Project Completion) review in January 2025 with early finish expected in April 2025.
- Linac Coherent Light Source II High Energy (SLAC): A combined CD-2/3 (Approve Performance Baseline/Approve Start of Construction) was approved on September 18, 2024.
- NSRC Recapitalization (multiple Labs): 16 of 18 instrument awards have been made, with 5 instruments delivered (2 installed).
- NSLS-II Experimental Tools-III (BNL): CD-1 (Approve Alternative Selection and Cost Range) approved on September 13, 2024.

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Space upstream of the existing Soft X-Ray (SXR) Undulator is prepared in August 2024 for the addition of nine LCLS-II-HE units.

APS-U First Light

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The upgraded APS achieved first light on June 17, 2024, with the resonant inelastic X-ray scattering program at 27-ID receiving the first X-rays.





Selected Recent Scientific Highlights





Attosecond Delays in X-ray Molecular Ionization

A team from the U.S., France, and the U.K. combined attosecond pulses from the LCLS with an intense circularly polarized IR laser field to measure up to a 700 attosecond delay in emission of electrons from different core-orbitals. Combined with theory, the work reveals the role that electron-electron interactions play in the observed delays. Ref.: Driver, et. al, *Nature*. (2024).

Decoding Imperfections in Hexagonal Boron Nitride (hBN) for Quantum Applications

By combining photoluminescence spectroscopy and resonant inelastic scattering at NSLS – II, researchers from BNL, CUNY, and NIMS (Japan) revealed how elementary excitations in defective hBN trigger harmonic electronic states that correlate with observed single photon emission. Ref.: Pelliciari, et. al, *Nature Materials*. (2024).



Selected Recent Scientific Highlights





Giant optical non-linearity of Fermi polarons in atomically thin semiconductors

Researchers from the U. Maryland, BNL, the MPI of Quantum Optics (Germany), and NIMS (Japan) demonstrated that a 2D device made of three atomic layers of WSe₂ could perform all-optical information processing using only a small number of photons. The approach shows promise for improving speed and energy efficiency of telecommunications and quantum communication Ref.: Gu, et. al, *Nature Photons*. (2024).

Solar-Driven Tandem Conversion of CO₂ to Butene

Researchers from the Liquid Sunlight Alliance, an Energy Innovation Hub, developed a tandem solar-driven electrochemical and photothermocatalytic process to convert CO_2 to butene using only simulated sunlight to drive the process. Analysis of the process demonstrated that the presence of H₂, CO, and H₂O leads to rapid deactivation of the Ni-based catalyst.

Ref.: Yap, et. al, ACS Energy Letters. (2024).



FY 2025 Request: \$2,582.3M (-\$43.3M or 1.65% below FY 2024 Enacted)

Research programs Δ = -\$18.1M

- Continued investments in research for clean energy, critical materials, FAIR and RENEW (+\$13M).
- Support for AI/ML increases (+\$8M), emphasizing research to accelerate discovery, translate large datasets into scientific understanding.
- Continued investments in microelectronics research, including networked team awards that comprise Microelectronics Science Research Centers.
- EFRCs, NQISRCs (recompeted/renewed), CMS/CCS, Fuels from Sunlight (renewal) and Batteries and Energy Storage Energy Innovation Hub awards, and DOE EPSCoR are flat funded.
- Expanded investments in SC Energy Earthshots initiative (+\$45M)

Scientific user facilities $\Delta = +$ \$81.4M

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- Operations of 12 facilities supported at 90% of funding required for re-baselined, normal operations (\$1,319.4M)
- Facilities research (\$60.9M): Accelerator & Detectors; AI/ML (+9M); BRaVE; preliminary planning for future MIEs



Construction/MIE Δ = -\$106.6M (includes OPC)

- LCLS-II-HE (\$100M); STS (\$52M); CRMF (\$20M); HFIR Pressure Vessel Replacement (\$11M); NEXT-III (\$10M)
- No Major Items of Equipment requested

BES Funding: Research, Facility Operations, Projects

FY 2025 President's Request is \$2,582M, \$43.3M (1.65%) below FY 2024 Enacted – balances major program components.

FY 2025 President's Request



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(\$K)	FY 2023 Enacted	FY 2024 Enacted	FY 2025 Request
Research	1,101,653	1,089,823	1,068,824
Facility Operations	1,068,647	1,235,177	1,319,461
Projects	362,700	299,625	193,000
GPP	1,000	1,000	1,000
Total	2,534,000	2,625,625	2,582,285



FY 2025 House and Senate Marks

- House Mark (June 28): \$2,617M (+\$34.3M or 1.3% above FY 2025 Request and -\$9M or 0.3% below FY 2024 Appropriation).
- Senate Mark (August 1): \$2,563M (-\$19.8M or 0.8% below FY 2025 Request and -\$63.1M or 2.4% below FY 2024 Appropriation). [In addition, Sen. Mark included \$100M for AI across SC]

		FY 2025	FY 2025	FY 2025	FY 2025 Pres.	FY 2025 Pres.
	FY 2024	President's	House	Senate	Req. vs House	Req. vs Senate
Basic Energy Sciences	Enacted	Request	Mark	Mark	Mark	Mark
Research	1,162,823	1,079,324	1,067,272	1,000,000	(12,052)	(79,324)
Facility Operations						
Light Sources	709,134	790,347	795,347	805,000	5,000	14,653
Neutron Sources	342,163	364,692	406,000	404,000	41,308	39,308
Nanoscale Science Research Centers (NSRCs)	150,880	164,422	164,422	170,000	-	5,578
	1,202,177	1,319,461	1,365,769	1,379,000	46,308	59,539
Projects						
Advanced Photon Source Upgrade (APS–U), ANL	-	-	-	-	-	-
Spallation Neutron Source Proton Power Upgrade (PPU), ORNL	15,769	-	-	-	-	-
Advanced Light Source Upgrade (ALS–U), LBNL	57,300	-	-	-	-	-
Linac Coherent Light Source-II—High Energy (LCLS—II—HE), SLAC	120,000	100,000	100,000	100,000	-	-
Second Target Station (STS), ORNL	52,000	52,000	52,000	52,000	-	-
Cryomodule Repair and Maintenance Facility	9,000	20,000	20,000	20,000	-	-
HFIR Pressure Vessel Replacement (PVR), ORNL	4,000	6,000	6,000	6,000	-	-
NSLS–II Experimental Tools—III (NEXT–III)	2,556	5,500	5,500	5,500	-	-
	260,625	183,500	183,500	183,500	-	-
Total, Basic Energy Sciences	2,625,625	2,582,285	2,616,541	2,562,500	34,256	(19,785)



Artificial Intelligence and Machine Learning (+\$17.4M, 60% above FY 2024 Enacted)

- AI for Science
 - Accelerate scientific discovery and realize broader insights from shared datasets
 - Develop surrogate models for expensive or timeconstrained experiments
 - Learn from multi-modal, sparse, and/or noisy data
- AI for User Facilities
 - Guided by BES Roundtable on Producing and Managing Large Scientific Data with AI/ML
 - Enhance efficiency of facility operations and design of experiments
 - Transform real-time analysis of data

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- Predict and mitigate instrument/facility down time (e.g., use of digital twins)
- Enable self-driving, autonomous instrumentation and experiments



Roundtable on Producing and Managing Large Scientific Data with Artificial Intelligence and Machine Learning







DOE-SC Roundtables: Transformational Science Enabled by Artificial Intelligence: October 28–31 & November 7–8, 2024



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SC Office Hours

- As part of the efforts to improve outreach and accessibility, SC is holding monthly virtual office hours to share information and provide opportunities to ask questions.
- Starting in September, the Office of Science (SC) is transitioning to one SC-wide monthly virtual Office Hour to share information about our programs and provide opportunities to ask questions.
- All are welcome to attend; no existing relationship with DOE or the DOE national laboratories is required. Research administrators are also encouraged to attend.
- Schedule and details are on the office hour page at <u>https://science.osti.gov/officehours</u>
 - Prior BES Office Hours (slides & video) available at https://science.osti.gov/bes/officehours
- Upcoming Office Hours and Topics:
 - Tuesday, October 1, 2024, at 2pm ET FY 2025 Annual Open Solicitation
 - Tuesday, November 12, 2024, at 2pm ET TBD
 - Tuesday, December 3, 2024, at 2pm ET TBD

THANK YOU!

Questions/Discussion

